even if amended herein or later during prosecution.

Claims 1 and 4-17 are all of the claims pending in the present Application.

Claims 1, 4-6, 15, and 16 stand rejected under 35 USC §102(e) as anticipated by US Patent 5,959,307 to Nakamura et al. Claims 9 and 17 stand rejected under 35 USC §102(b) as anticipated by US Patent 5,777,350 to Nakamura et al. Claims 7, 8, and 10-14 stand rejected under 35 USC §102(e) as anticipated by or, in the alternative, under 35 USC §103(a) as unpatentable over US Patent 5,959,307 to Nakamura et al.

These rejections are respectfully traversed in view of the following discussion.

I. The Claimed Invention

As described and claimed, for example by claim 1, the present invention is directed to a group III nitride compound semiconductor light-emitting device including a light-emitting layer of a multilayer quantum well structure including alternately laminated well layers and barrier layers and an n-type clad layer being in contact with the light-emitting layer. The n-type clad layer is made thicker than each of the barrier layers and the thickness of the n-type clad layer is in a range of 100 Å to 500 Å. The n-type clad layer is formed of a material substantially the same as the barrier layers, thereby providing a band gap in the n-type clad layer that is substantially the same as a band gap in the barrier layers.

With such unique and unobvious features, high light intensity is provided by securing the effect of confining carriers sufficiently in the light-emitting layer while keeping color purity intact.

This aspect of color purity is significant in the art. The present invention has high color purity by forming barrier layers and a clad layer with essentially the same materials,

thereby band gaps of these layer are essentially equal.

A band gap in the well layer depends on the thickness of the barrier layer and the thickness of the well layer, as represented by the Kronig & Penny model shown in Equation (1) in the attached Appendix I (Lb: thickness of barrier layer; Lz: thickness of the well layer). For the Examiner's convenience, this equation is explained in detail in the attached Appendix II "Introduction for Solid-State Physics", on page 243 and 245 (11-19).

The energy level of the well layer is determined by these factors, so it is not easy to enhance the color purity of the emitted light.

For example, US Patent 5,959,307 to Nakamura discloses an AlGaN layer 201 formed just below the first well layer, which is different from the GaN barrier layer. In this case, a larger compression strain is applied to the first well layer, as compared to the present invention. This strain affects the band gap of the first well layer, and more specifically, reduces the band gap and, thereby, increases the wavelength of the emitted light.

The relationship of the lattice constant is InGaN > GaN > AlGaN. In Nakamura, the first well layer InGaN (column 6, line 15-16) is sandwiched between the n-clad layer AlGaN 201 with a small lattice constant and the barrier layer GaN with middle lattice constant. Therefore, the compression strain acting on the first well layer is made larger.

Even though assuming arguendo that the possibility of using AlGaN as the barrier layer is alluded to in column 6, line 29, there is no suggestion in Nakamura that color purity depends upon using the same materials. Therefore, without some indication in Nakamura that the problem of color purity can be addressed by using the same materials, Applicants respectfully submit that one of ordinary skill in the art would consider that Nakamura actually teaches against the concept of the present invention that the band gap of the n-type clad layer

is made essentially equal to the band gap of the barrier layer, particularly in view of the levels shown in Figure 5 of Nakamura.

II. The New Prior Art Rejection Based on Nakamura '350

The Examiner maintains the rejection based on US Patent 5,959,307 to Nakamura et al., as modified to incorporate a new rejection based on US Patent 5,777, 350 to Nakamura et al. In this section, Applicants respond to this latest rejection based on Nakamura '350.

Moreover, although Applicants have responded to the rejection based on Nakamura '307, in Section IV below, in order to allow the Examiner to update this somewhat dated rejection in view of the following discussion for the latest rejection, a listing of perceived deficiencies for the Nakamura '307 rejection is provided.

In the Office Action dated August 6, 2003, the Examiner alleges that Nakamura '350 anticipates the present invention as described by claims 9 and 17. However, Applicants respectfully disagree.

A key feature of the present invention, as defined by claim 1, is that, as described by lines 3-5 of page 9 of the specification, the barrier layers and n-type clad layer are made of substantially the same material, by reason that the barrier layers are formed using "the same condition as used for forming the n-type clad layer".

Applicants again respectfully submit that the rejections of record based on either Nakamura reference possesses a basic flaw that must be properly addressed prior to proceeding to appeal.

More specifically, the rejection of record merely observes that the statements in both references leaves open the possibility of the combination of elements defined by the claims of

the present invention.

That is, contrary to the allegations in the rejections of record, a <u>fair and reasonable</u> reading of these references clearly demonstrate that there is <u>no suggestion whatsoever</u> in either reference to <u>construct the barrier layer to be essentially identical to the n clad layer adjacent to the active layer</u>.

The Examiner merely points to a statement of possible components and then confuses the <u>possibility inherent in this potential list of components</u> as constituting either a teaching or a suggestion to make the claimed combination.

As Applicants have already pointed out on the record, this approach in the rejections of record <u>violates the guideline</u> in MPEP §2143.01: "The mere fact that references <u>can</u> be combined or modified does not render the resultant combination obvious unless the prior art also suggests the desirability of the combination" (emphasis in MPEP).

The present invention is <u>clearly a new combination of elements</u>, even if these elements can be found in isolation, based on a listing of potential components and/or ranges in a prior art reference. That is, the present invention teaches that having <u>essentially identical composition for the barrier layers and adjacent n-clad layer</u> provides a significant advantage.

The new rejection based on Nakamura '350 <u>raises exactly the same issues</u> presented by the rejection based on Nakamura '307 in that the Examiner points to a listing of possible components and concludes that, by reason that the <u>possibility exists in Nakamura '307 to re-combine elements differently than explicitly described therein</u>, the reference anticipates the new combination of elements defined by present invention. However, it is totally irrelevant that the present invention <u>*could*</u> be reconstructed from the ranges and possible components in Nakamura '350 (or Nakamura '307), given the advantage of having read the present

specification.

More specifically, even if all allegations in Paragraphs 3 and 3a of page 2 of the Office Action dated August 6, 2003, were correct, it remains incorrect to allege that Nakamura '307 teaches the use of substantially the same material for the barrier layer and the first n-clad layer. That statement is nowhere to be found in Nakamura '307. It is the Examiner, not the prior art reference, who makes this combination.

Moreover, relative to claims 9 and 17, in Paragraph 3b on page 3 of the Office Action, the Examiner further concludes that the express teaching to use a substantially different material for the cap layer "... does not teach away from using GaN for the cap/clad. Rather, the reference teaches that using GaN was known, but that AlGaN is better."

Applicants submit that the Examiner's above description of Nakamura '350 can only be interpreted as expressly teaching away from using GaN as an element.

III. The Prior Art Rejections Currently of Record Use Incorrect Legal Standards and Incorrectly Apply the Facts in the Nakamura References

The underlying basic flaw in the rejections of record is that the Examiner applies a number of incorrect legal standards.

First, for anticipation, a single reference must teach every element of the claim (e.g., see MPEP §2131). That is, the Federal Circuit has repeatedly emphasized that anticipation is established only if (1) all the elements of an invention, as stated in a patent claim, (2) are identically set forth, (3) in a single prior art reference.

In the present Application, the Examiner continues to maintain that Nakamura '307 and Nakamura '350 both teach the claim limitation of independent claims 1 and 15. To do so,

each reference must teach:

- a light-emitting layer having a multilayer quantum well with barrier layers; and

- an n-type clad layer in direct contact with the light-emitting layer that is thicker than the barrier layers and that is formed of substantially the same material as that of the barrier layer.

However, as previously pointed out, none of the three embodiments shown in Figures 2, 3, and 4 of Nakamura '307 and none of the 15 examples described in columns 14-18 teach (or even suggest) using an n-type clad layer in direct contact with the light-emitting layer that is formed of substantially the same material as that of the barrier layer.

It is the Examiner who alleges that Nakamura could be modified to satisfy this claim limitation.

Similarly, there is no teaching or suggestion in Nakamura '350 that the barrier layers and the n-type clad layer adjacent to the light-emitting layer be formed of substantially the same material in any of the nine embodiments shown in Figures 1-16 and described in columns 6-34. Nor do any of Example 1 through Example 27 teach or suggest this claim limitation. Indeed, most of the examples in Nakamura do not even have barrier layers of a multilayer quantum well and use, instead the single-quantum well structure.

Again, it is the Examiner who alleges that Nakamura '350 could be modified because elements are considered as being known in the art. Furthermore, it is noted that the Examiner cites and applys Nakamura after a close and thorough reading of Applicants' own specification.

As best understood, the Examiner's reasoning in an anticipatory rejection under 35 USC §102 is that, if a possibility exists to modify the reference in a manner not suggested in

that reference, the mere possibility of such modification satisfies as being an express or inherent teaching.

That reasoning is not the legal standard. The Examiner has the initial burden to point out explicitly each claim limitation in a rejection under 35 USC §102. If that reference must be further modified to satisfy the limitation, then the Examiner has the burden to proceed with a rejection analysis under 35 USC §103, rather than anticipation.

That is, in the present Application, the rejection of record does not point to an express teaching anything in the two references to justify that "substantially the same material" is used for both barrier layers and the adjacent n-clad layer. (As discussed above, the Nakamura references are clearly deficient in teaching or suggesting this limitation.) Instead, the rejection declares that the limitation would be satisfied if the embodiments described were further modified to incorporate a structure not expressly described but which would be possible if one or more generalized statements were to be implemented in accordance with the claim limitation.

Second, the Examiner further alleges that the ranges recited in various claims are additionally obvious because these ranges fall within or overlap ranges recited in Nakamura '307.

There are at least two underlying basic problems with this analysis of ranges. First, as described in MPEP §2131.03, each range must be analyzed to determine if

> *"... the claimed subject matter [is] disclosed in the reference with 'sufficient specificity to constitute an anticipation under the statute'.... If the claims are directed to a narrow range, the reference teaches a broad range, and there is evidence of unexpected results within the claimed narrow range, depending on the other facts of the case, it may be reasonable to conclude that the narrow range is not disclosed with 'sufficient specificity' to constitute an anticipation of the claims. The unexpected results may also render the claims unobvious."*

Applicants submit that the rejection currently of record fails to take the above-identified approach of MPEP §2131.03. The rejection fails to properly address the claimed narrower ranges, which Applicants consider as providing optimum ranges rather than the broad ranges mentioned in Nakamura.

Second, Applicants have stated on the record that the ranges recited in the claims, in combination with the limitations of independent claim 1, provides the unexpected result of high light intensity while keeping color purity intact. That is, considering even claim 1 alone, the present invention combines the aspect of confining carriers in the n-clad layer by using thickness, rather than band gap, the present invention provides a crystal interface at the n-clad interface that improves color purity and intensity.

The other recited ranges of other parameters improve the intensity of these two effects. Thus, Applicants submit that the Examiner's reliance, in paragraph 4.b.iv. on page 5 of the Office Action on *In re Luck* is misplaced. That is, Applicants submit that there is an unexpected result achieved in combining even the elements of claim 1.

The Examiner attempts, in Paragraph 6a on page 8 of the Office Action dated August 6, 2003, to characterize this unexpected result as being "... *another advantage which would flow naturally from following the suggestions of the prior art.*"

Applicants submit that the problem with the Examiner's characterization is that the Nakamura references fail to teach or even suggest the combination of elements described in claim 1. It is the Examiner who suggests that these references could be modified as described in claim 1. Thus, unless the Nakamura references teach the specific combination defined in claim 1, there cannot possibly be "another advantage which would flow naturally" from Nakamura.

The Examiner relies upon Ex parte Lee (Board of Patent Appeals and Interferences), 31 USPQ2d 1105 (1993), to justify the approach in the rejection of record for ranges. This reliance on Lee is also misplaced, since that decision involved a case in which the invention was identical in all other respects except a single variable which fell within a range described in the reference.

In contrast, in the present invention, Applicants traverse that the Nakamura references even suggest the limitation of having substantially same material for the barrier layers and the adjacent n-clad layer of the independent claim 1, let alone the substantially same material for a cap layer on the side of the active layer opposite the n-clad layer, as additionally required by dependent claim 9, which claim 9 is further the basis for claims 10-14.

In contrast to the facts of Lee, the claims of the present invention describe a combination of ranges of different parameters. For example, claim 1 addresses the thickness range of the n-type clad layer, claims 5 and 6 address ranges of ratio of elements in the intermediate layer, claim 8 address relative thicknesses of the barrier layer and the well layer, claims 10-13 address the thickness of the p-type clad layer, and claim 14 addresses the range of ratio of elements in the p-type clad layer.

Stated differently, these claims describe a successively more complex combination of elements that is conjunctively interconnected. The Examiner has the initial burden to reject the combination of ranges of the different parameters as a cumulative combination of elements. This approach is not taken in the rejection of record. Instead, the rejection relies on assuming that narrow ranges are inherently included in broader ranges of the references and, therefore, obvious.

Applicants submit that the appropriate legal standard appropriate to the analysis of the

present Application is better defined in MPEP §2144.05 II. B. in which section it is described that each "... *particular parameter must first be recognized as a result-effective variable, i.e., a variable which achieves a recognized result, before the determination of the optimum or workable ranges of said variables might be characterized as routine experimentation* (emphasis by Applicants)." This section is citing *In re Antonie*, 559 F.2d 618, 195 USPQ 6 (CCPA, 1977).

The following words from that case would seem an appropriate criticism of the technique of the rejection currently of record, as follows (emphasis by Applicants):

> *"In determining whether the invention as a [whole] would have been obvious under 35 U.S.C. §103, we must first delineate the invention as a whole.... Just as we look to a chemical and its properties when we examine the obviousness of a composition of matter claim, it is this invention as a whole, and not some part of it, which must be obvious under 35 U.S.C. §103.... The PTO and the minority appear to argue that it would always be obvious for one of ordinary skill in the art to try varying every parameter of a system in order to optimize the effectiveness of the system even if there is no evidence in the record that the prior art recognized that particular parameter affected the result. As we have said many times, obvious to try is not the standard of 35 U.S.C. §103.... Disregard for the unobviousness of the results of 'obvious to try' experiments disregards the 'invention as a whole' concept of § 103,.... and over-emphasis on the routine nature of the data gathering required to arrive at appellant's discovery, after its existence become[s] expected, overlooks the last sentence of §103. "*

That is, in the two prior art Nakamura references, there are, taken together, 12 embodiments and 42 examples. These embodiments and examples present a variety of different values and combinations to provide a variety of parameters that include composition, ranges of composition, thicknesses of various layers, and absence of some layers in some configurations.

None of the embodiments/examples of these two references provide a single example, or makes a suggestion, or even recognizes the *possible* significance of the parameter that the

barrier layer and the n-clad layer composition be identical (e.g., "substantially the same material"). That is, none of the 12 embodiments or the 42 examples in the two Nakamura references provide even a suggestion that this parameter might be significant in any way.

It is the present invention that identifies the significance of this parameter of common composition.

As previously explained on the record, this feature of the present invention in which the barrier layer and n-type clad are the same material provides colorimetric purity of the emitted light. If the barrier layer and n-type clad differ in material, then the lattice constants of these layers will also differ.

It makes a difference between the strain imposed on the lowermost well layer adjacent to the n-clad layer and the strain on the other well layers. As shown in Figure 1 of the present Application, there are three well layers 161, and the quantum level of the lowermost well layer differs from that of other layers. Each of the well layers respectively emits light, but the color of the light (wavelength) from the lowermost well layer would differ from light emitted from the other two layers due to the difference of the strain, if strain were not matched, since it is known that such strain affects the quantum level of the layer.

That is, only the lowermost well layer among the three well layers is adjacent to the n-clad layer on one side opposite to the barrier layer. Accordingly, if the n-clad layer is made of different material from the barrier layer, then the quantum level state on respective sides of the lowermost well layer would be asymmetric, thereby affecting the quantum level of the well layer itself, which exists between two layers.

The total light is a mixture of the three light emissions from the three respective light well layers. Accordingly, colorimetric purity of the total light is deteriorated if the n-clad layer

is made from material different from that of the barrier layer.

In contrast, in the present invention, substantially the same material is used for the barrier and n-type clad, thereby <u>making equal the strain on each well layer and making symmetric the quantum level on both sides of the lowermost well</u>. As a result, colorimetric purity of the total light can be maintained in the present invention. No such feature of the n type cladding layer and the barrier layers being formed of substantially the same material is suggested in Nakamura.

IV. Specific Deficiencies of the Claim Rejections Currently of Record

To summarize the deficiencies of the rejections currently of record, Applicants submit the following listing to permit the Examiner to address this listing on the record prior to proceeding to appeal.

<u>Relative to claims 1 and 15</u>, the rejection of record is deficient for the following reasons:

1. As pointed out above, neither Nakamura '307 nor Nakamura '350 teaches or even reasonably suggests using substantially the same materials for the n-clad and the barrier layers. The fact that the materials listed therein would <u>allow the combination</u> is irrelevant, unless the Examiner can demonstrate a reasonably proper motivation. That is, this limitation is a very narrow limitation of the broad ranges of compositions/potential combinations of compositions listed in Nakamura. Applicants have stated the significance on the record of this parameter and that it provides an unexpected result.

Hence, turning to the clear language of the claims, there is no teaching or suggestion that " ... said n-type clad layer is formed of a <u>material substantially the same</u> as said barrier layers, thereby providing a <u>band gap in said n-type clad layer that is substantially the same as a</u>

band gap in said barrier layers."

Relative to Claim 6:

1. This claim defines a narrow range for the intermediate layer $In_xGa_{1-x}N$, where $0.01 \leq x \leq 0.05$. The significance of this narrow range, in combination with the limitations of claim 1, is explained on page 5 at lines 3-16. That is, an acute intensity peak occurs when this intermediate has a ratio x of approximately 0.03. When x is above 0.05, the crystallinity deteriorates and when x is below 0.01, the intensity decreases.

2. The rejection currently of record fails to properly address this narrow limitation, either alone or in combination with the elements of claim 1. It is noted that the narrow range provide the unexpected result identified above in (1), so that a proper rejection would have to address the narrow range, rather than merely assert that the narrow range is included in a broader range.

Hence, turning to the clear language of the claims, there is no teaching or suggestion that " ... where ($0.01 \leq x \leq 0.05$)."

Relative to Claims 7 and 16:

1. The rejection currently of record shows that GaN is included in a listing of potential components for the barrier layers and in a listing of potential components for the n-clad. No where does the rejection show an example or statement in Nakamura '307 or '350 that GaN is desired to be used together in the same device.

2. Because of this deficiency, neither Nakamura reference reasonably can be considered as anticipating this limitation. The Examiner has an initial burden to demonstrate a motivation to modify one of these two references.

Hence, turning to the clear language of the claims, there is no teaching or suggestion

that " ... wherein said n-type clad layer and said barrier layers are formed of GaN."

Relative to claim 8:

1. This claim contains a limitation that two parameters have, respectively, specific values. The barrier thickness is significant relative to the thickness of the n-clad layer, as identified in claim 1.

2. Therefore, the Examiner has the initial burden to demonstrate that this very narrow range of not only one parameter, but two parameters in combination, is taught or reasonably suggested in Nakamura '307. This burden is more than merely a statement that the broad ranges of these parameters in Nakamura covers this claimed range, as is currently done in the rejection (e.g., see MPEP §2144.05 II B: "A particular parameter must first be recognized as a result-effective variable, i.e., a variable which achieves a recognized result, before the determination of the optimum or workable ranges of said variables might be characterized as routine experimentation.").

Hence, turning to the clear language of the claims, there is no teaching or suggestion that " ...wherein a thickness of said well layer is approximately 30 Å and a thickness of said barrier layer is approximately 70 Å".

Relative to claims 9 and 17:

1. Contrary to the Examiner's allegation, Nakamura '350 does not teach a configuration matching the description of claim 1 in which the barrier layers are stated to be GaN, and the n-clad layer is stated as also being GaN, and the thickness of the n-clad layer is greater than that of the barrier layers. The ranges and listing of components provide, at most, the possibility of the described configuration. As pointed out above, Nakamura does not recognize the significance of having the same composition for the barrier layers and n-clad

layer.

2. Therefore, Nakamura '350 does not anticipate claim 1, and the Examiner has an initial burden to provide a reasonable burden to modify it.

3. Further, relative to claims 9 and 17, Nakamura does teach against using GaN as the first p-clad layer 61. The Examiner would have the initial burden of overcoming this express preference in Nakamura.

Hence, turning to the clear language of the claims, there is no teaching or suggestion that "... a cap layer formed on said light-emitting layer, said cap layer being formed of a material substantially the same as said barrier layers."

Relative to Claim 10-13:

The significance of the optimal thickness of the p-type clad is discussed at line 16 of page 11 through line 5 of page 12. Nakamura does not recognize the significance of the p-clad layer as related to optimal intensity for various wavelengths. Therefore, under MPEP §2144.05 II B, the Examiner has the initial burden of establishing a reasonable rejection for the narrower range claimed in the present invention.

Hence, turning to the clear language of the claims, there is no teaching or suggestion that "... wherein a thickness of said p-type clad layer is in a range of approximately 180 Å to 500 Å, and a light emitted comprises green light in a wavelength range of approximately 510 nm to 530 nm", "... wherein said thickness of said p-type clad layer is in a range of approximately 240 Å to 360 Å", "... wherein a thickness of said p-type clad layer is in a range of approximately 90 Å to 390 Å, and a light emitted comprises blue light in a wavelength range of approximately 460 nm to 475 nm", and ".... wherein said thickness of said p-type clad layer is in a range of approximately 120 Å to 300 Å".

<u>Relative to claim 14</u>:

. The significance of the optimal composition range for the p-clad layer is discussed at lines 6-14 of page 12. If x is smaller than 0.10, the light emission is lowered because it is difficult to confine carriers in the light-emitting layer. If x is greater than 0.14, the light emission output is lowered due to stress. Therefore, under MPEP §2144.05 II B, the Examiner has the initial burden of establishing a reasonable rejection for the narrower range claimed in the present invention.

Hence, turning to the clear language of the claims, there is no teaching or suggestion that "... wherein said p-type clad layer comprises p-type doped $Al_xGa_{1-x}N$, where x ranges from approximately 0.10 to 0.14."

For the reasons stated above, the claimed invention is fully patentable over the cited reference.

Further, the other prior art of record has been reviewed, but it too even in combination with the two Nakamura references, fails to teach or suggest the claimed invention.

V. Formal matters and Conclusion

In view of the foregoing, Applicant submits that claims 1 and 4-17, all the claims presently pending in the application, are patentably distinct over the prior art of record and are in condition for allowance. The Examiner is respectfully requested to pass the above application to issue at the earliest possible time.

Should the Examiner find the application to be other than in condition for allowance, the Examiner is requested to contact the undersigned at the local telephone number listed below to discuss any other changes deemed necessary in a <u>telephonic or personal interview</u>.

The Commissioner is hereby authorized to charge any deficiency in fees or to credit any overpayment in fees to Attorney's Deposit Account No. 50-0481.

Respectfully Submitted,

Date: 10/31/03

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Attachments:
- Attachment I (1 page)
- Attachment II (5 pages)

Appendix I

文献 ELECTRONICS LETTERS Vol. 18, No. 6, p. 227~229 (1983) (著者 K. ALAVI, T. P. PEASALL et al.) に記載の

バリア層：$Al_{0.48}In_{0.52}As$，井戸層：$Ga_{0.47}In_{0.53}As$から成るMQW（多重量子井戸）構造を有する発光ダイオードにおいて，井戸中に形成される離散したエネルギーレベルの最も高いエネルギーレベルの位置が，バリア層のコンダクションバンドの底と一致しているかどうかを計算により確認する

【計算をサポートする理論】

①周期的な凹凸を有するポテンシャル中の電子（又は正孔）の挙動はクローニッヒ・ペニイの模型を用いて厳密に記述することができる.

②井戸中に形成されるエネルギーレベルは，クローニッヒ・ペニイの模型（詳細は添付資料6を参照）によれば，以下のように表される.

$$[(\beta^2-\alpha^2)/2\alpha\beta]\sin h\beta L_b \sin\alpha L_z + \cos h\beta L_b \cos\alpha L_z = \cos k(L_z+L_b) \quad \cdots\cdots (1)$$

ここで，L_bはバリア層の厚さ，L_zは井戸層の厚さである.

αおよびβは，電子のエネルギーE及びポテンシャルバリアの高さV_0を用いて次のように表される.

$$\alpha=(2m\cdot E/\hbar^2)^{1/2},\quad \beta=\{2m\cdot(V_0-E)/\hbar^2\}^{1/2} \quad \cdots\cdots (2)$$

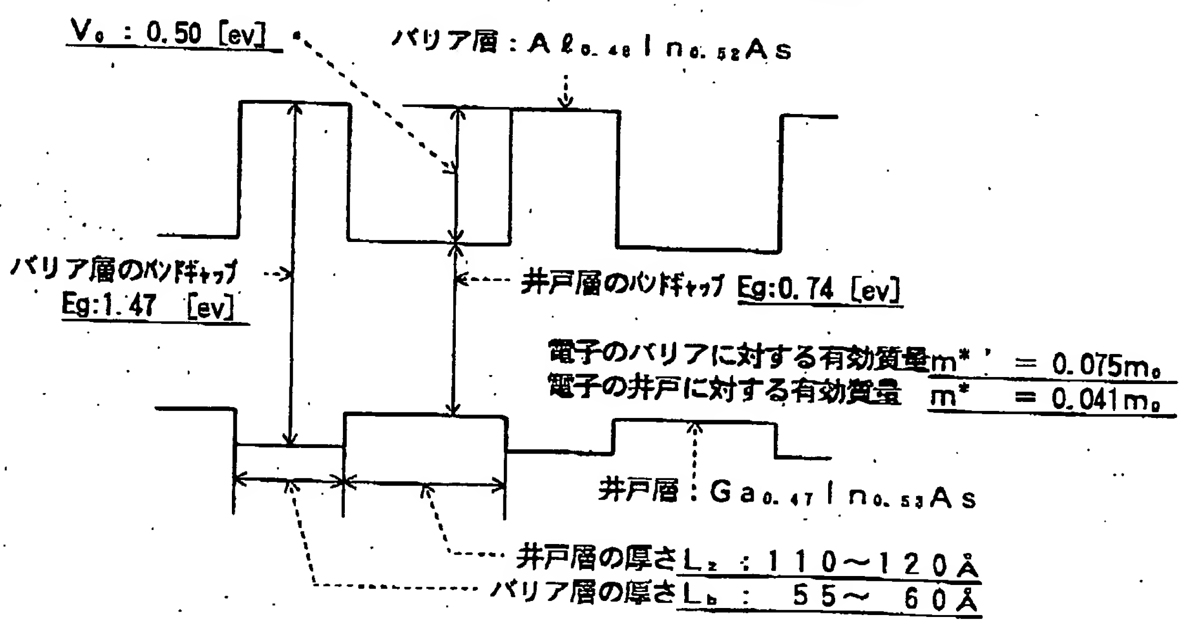
また，kは電子の波数である。

kが実数であるためには，式(1)の右辺の絶対値，即ち，$|\cos k(L_z+L_b)|\leqq 1$であるから，井戸中に形成されるエネルギーレベルは，以下の式が満たされる場合に存在する.

$$\boxed{|[(\beta^2-\alpha^2)/2\alpha\beta]\sin h\beta L_b \sin\alpha L_z + \cos h\beta L_b \cos\alpha L_z| \leqq 1 \quad \cdots\cdots (3)}$$

③今回の場合はポテンシャルバリア層である$Al_{0.48}In_{0.52}As$の厚さL_bが薄いため，ポテンシャルバリア層（$Al_{0.48}In_{0.52}As$）を挟んだ隣り合う量子井戸層（$Ga_{0.47}In_{0.53}As$）の電子の波動関数どうしが重なり合うようになり，井戸形ポテンシャルが単独に存在するとして取り扱った場合には縮退していた量子準位がトンネル効果により分裂し，いわゆるミニバンドと呼ばれるエネルギー帯が形成されることを考慮する必要があるが，これに関してもクローニッヒ・ペニイの模型が適用できる。従って，今回の計算に関しては，式(3)を適用することができる。

【式(3)による計算を行うに際し，文献内に記載されているパラメータの確認】



Appendix II

互に離れているために内部の波動函数の重なりが殆とんどないからである．狭くてエネルギーが低いバンドは，外側の空いたバンドや部分的に満ちたバンドとはそのエネルギーが重なり合わない．また閉殻は常に偶数個の電子を含むから，これに対するエネルギーバンドも満ちている．

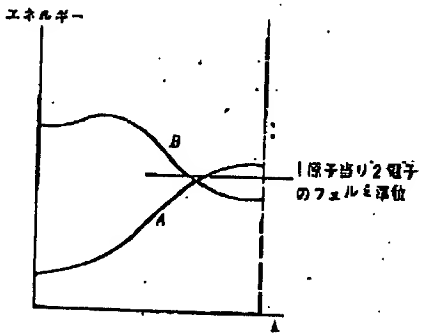


図 11・6 A，B のエネルギーバンドの重なりを示す．これは二価金属の金属伝導性の説明図である．図のように各バンドはフェルミ面まで満ちているが，A は完全には満ちていず，また B も少し電力を含んでいる．重なりは同バンドで同一方向の k で起る必要はない．

固体が絶縁体となるためには，原子あるいは単位胞が偶数の電子を含むことが必要であり，さらに最も外側の満たされたエネルギーバンドが，問題とする温度で kT よりもずっと大きいエネルギー間隔だけ他のバンドより下になければならない．アルカリ土類金属は2価だけれども図 11・6 に示すようにエネルギーバンドが重なり合っているために絶縁物ではない．このように，重なりがなければ完全に満ちるはずのエネルギーバンドもこのため完全には満ちず，また重なりがなければあいているはずのバンドも部分的に満ちていることになる．アルカリ金属と貴金属は，これらが一価金属であって，かつエネルギーバンドが半分だけ満ちているために良導体である．ダイヤモンドは4個の価電子を含み，問題となる空のエネルギーバンドとは約 5 eV はなれているから絶縁体である．ケイ素とゲルマニウムはダイヤモンドと同一構造で，等しい原子価をもっているが半導体である．これらでは上述のエネルギー間隔が 1 eV の程度しかないからである．食塩は絶縁体であって，格子点一つ当りの NaCl の電子数は 28 であり偶数である．絶縁体と金属伝導体との本質的な違いは，このように原子価の違いならびに各エネルギーバンド間のエネルギーの関係の相違にある．

周期格子中の波動函数

ブロッホ[3] は重要な定理すなわち "周期的なポテンシャルをもつシュレーディンガー方程式の解は

$$\psi_{\mathbf{k}} = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \qquad (11\cdot3)$$

3) F. Bloch, Z. Physik 52, 555 (1928); この結果は数学者には早くから Floquet の定理として知られていた．

という形をしている" という定理を証明した．ここに $u_{\mathbf{k}}(\mathbf{r})$ は一般には $\mathbf{k}$ の函数であって，ポテンシャルの周期すなわち格子の周期をもつ x, y, z の周期函数である．この形から平面波 $e^{i\mathbf{k}\cdot\mathbf{r}}$ が格子の周期で変調されていることがわかる．(11・3) 式の解はブロッホ函数として知られている．

ブロッホの結果の模型的な証明はモットとジョーンズの著書の 57〜59 頁に与えられている．ブロッホ自身は初等的な群論をもちいてもっと満足な証明を与えている．ここに示すのは簡単にしたやや不完全な要約である．長さ Na の円環の上に N 個の格子点を考え，ポテンシャルは周期 a をもつものとする．そこで g を整数とするときは次式が成立する．

$$V(x) = V(x + ga) \qquad (11\cdot4)$$

円環の対称性を満すように，C を定数として

$$\psi(x + a) = C\psi(x) \qquad (11\cdot5)$$

のような性質をもった固有函数を求めよう．すると

$$\psi(x + ga) = C^g\psi(x) \qquad (11\cdot6)$$

となる．固有函数は一価函数であるはずであるから

$$\psi(x + Na) = \psi(x) = C^N\psi(x) \qquad (11\cdot7)$$

となり，C は1の N 乗根の一つでなければならない．すなわち，

$$C = e^{i2\pi g/N};\ g = 0,\ 1,\ 2, \ldots\ldots, (N-1). \qquad (11\cdot8)$$

したがって

$$\psi(x) = e^{i2\pi xg/Na}u_g(x) \qquad (11\cdot9)$$

は $u_g(x)$ が a の周期をもつならば，満足な解である．

いま

$$k = 2\pi g/Na \qquad (11\cdot10)$$

と置けば，ψ はつぎのようになる．

$$\psi_k = e^{ikx}u_k(x) \qquad (11\cdot11)$$

これがブロッホの結果である．

クローニッヒ・ペニイの模型

簡単な模型をもちいて，結晶内を電子が伝播するときのいくつかの特徴を示そう．モデルとして，一次元の周期的な井戸型ポテンシャル (図 11・7) を考える[4]．これはひどく

4) R. de L. Kronig and W. G. Penney, Proc. Roy. Soc., (London) A130, 499 (1931); また D.S. Saxon and R.A. Hutner, Philips Research Repts. 4, 81 (1949); J. M. Luttinger, Philips Research Repts. 6, 303 (1951) をみよ．

人為的な模型であるが初等函数だけを用いて具体的に取扱える長所がある．さて問題の波動方程式は，

(11・12)　$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}(E-V)\psi=0$$

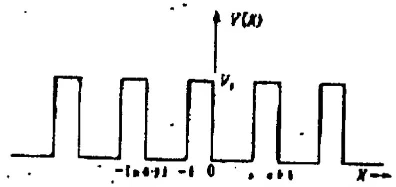


図 11・7　クローニッヒ・ペニイの一次元周期ポテンシャル

である．進行波の解は格子の周期で変調された平面波の形をしている．平面波に対して (11・11) 式をもちいて，つぎの形の解を求める．

(11・13)　$$\psi=u_k(x)e^{ikx}$$

ここに $u(x)$ は周期 $(a+b)$ をもった x の周期函数である．(11・13) 式を (11・12) 式に代入すると $u(x)$ を決定するつぎの方程式を得る．

(11・14)　$$\frac{d^2u}{dx^2}+2ik\frac{du}{dx}+\frac{2m}{\hbar^2}(E-E_k-V)u=0$$

ここに $E_k=\hbar^2k^2/2m$.

領域 $0<x<a$ で，この方程式はつぎの解をもつ．

(11・15)　$$u=Ae^{i(\alpha-k)x}+Be^{-i(\alpha+k)x}$$

ただし

(11・16)　$$\alpha=(2mE/\hbar^2)^{1/2}$$

領域 $a<x<a+b$ では，解は

(11・17)　$$u=Ce^{(\beta-ik)x}+De^{-(\beta+ik)x}$$

である．ただし

(11・18)　$$\beta=[2m(V_0-E)/\hbar^2]^{1/2}$$

定数 A, B, C, D は u と du/dx が $x=0$ と $x=a$ で連続であるようにえらばなければならない．また $u(x)$ は周期的であるという要請から $x=a$ における u の値は $x=-b$ における値と等しくなければならない．この条件を用いて，われわれは4個の線形同次方程式を得る．

$$A+B=C+D;$$
$$i(\alpha-k)A-i(\alpha+k)B=(\beta-ik)C-(\beta+ik)D;$$
$$Ae^{i(\alpha-k)a}+Be^{-i(\alpha+k)a}=Ce^{-(\beta-ik)b}+De^{(\beta+ik)b};$$
$$i(\alpha-k)Ae^{i(\alpha-k)a}-i(\alpha+k)Be^{-i(\alpha+k)a}=(\beta-ik)Ce^{-(\beta-ik)b}-(\beta+ik)De^{(\beta+ik)b}$$

これらの方程式は係数からつくられる行列式が零になるときだけ解がある[5]，すなわち

$$\frac{\beta^2-\alpha^2}{2\alpha\beta}\sinh\beta b\sin\alpha a+\cosh\beta b\cos\alpha a=\cos k(a+b).\qquad(11\cdot19)$$

この式はやや複雑であるので，もっと手頃な式を得るために，ポテンシャルを周期的なデルタ函数であるとする：すなわち，$b=0$ の極限で V_0 は β^2b が有限に留るような仕方で無限大 $(V_0=\infty)$ となるものとする．

$$\lim_{\substack{b\to0\\ \beta\to\infty}}\frac{\beta^2ab}{2}=P\qquad(11\cdot20)$$

とおくと，条件 (11・19) 式はつぎのようになる．

$$P\frac{\sin\alpha a}{\alpha a}+\cos\alpha a=\cos ka\qquad(11\cdot21)$$

(11・13) 式の形の波動函数が存在するためには，この超越方程式が α について解をもたなければならない．

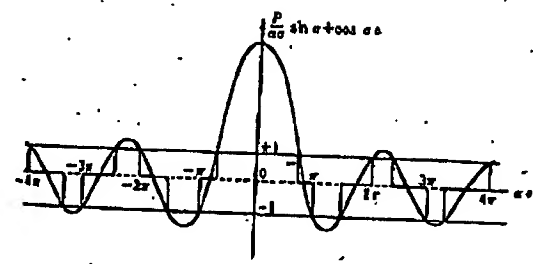


図 11・8　函数 $P\dfrac{\sin\alpha a}{\alpha a}+\cos\alpha a$ ($P=3\pi/2$ の場合) の図．函数の値が $+1$ と -1 の間にあるような $\alpha=[2mE/\hbar^2]^{1/2}$ の領域に対応するエネルギー E の値が許される．(Kronig と Penney による)

図 11・8 に (11・21) 式の左辺を αa の函数として図示した．ただしここでは P の値として任意に $3\pi/2$ とした．左辺の cos 函数は $+1$ と -1 との間の値をとるから，左辺の値がこの領域に入るような αa 値だけが許されることになる．αa の許される領域は図中で太い線で記してある．そして $\alpha=[2mE/\hbar^2]^{1/2}$ という関係により α の許される領域がエネルギー E の許される領域に対応している．αa の許容領域の境界は，k の値の $n\pi/a$ に対応する．図 11・9 には E を k の函数として示してある．

5) このことを自分自身で証明する前に，読者は次節に記されているクローニッヒ・ペニイの結果の別の導き方を参照すること．

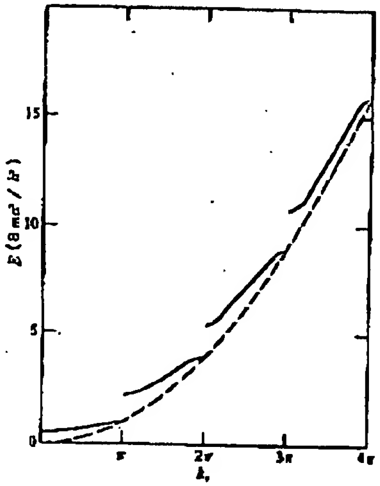


図 11・9 クローニッヒ・ペニイのポテンシャルに対してエネルギーと波数との関係．$P=3\pi/2$ の場合を画く．(Sommerfeld と Bethe による)

もし P が小さければ，禁止された領域がなくなる．もし $P\to\infty$ となれば，αa の許される領域は一列の点（$n=\pm1,\pm2\cdots\cdots$）に縮まってしまう．そのときにはエネルギー・スペクトルは離散的となり，固有値

$$E=n^2h^2/8ma^2$$

は長さ a の箱の中に閉じこめられた電子の固有値と一致する．

クローニッヒ・ペニイの結果の別解法

ここでは (11・19) 式に伴うかなりの労力を避けて，一列のデルタ函数のポテンシャルに対して，直接に結果 (11・21) 式を導こう．初めにデルタ函数のところで $\beta\gg k$ の領域に注目すると，その領域では d^2u/dx^2 は du/dx よりもはるかに大きい．われわれの境界条件はこのときにはデルタ函数型ポテンシャルの極限において u の値がポテンシャルを通して連続であるということになる．または周期条件を用いて

$$A+B\cong Ae^{i(\alpha-k)a}+Be^{-i(\alpha+k)a} \tag{11・22}$$

さらに，導函数はつぎの式で結びつけられる．

$$\left(\frac{du}{dx}\right)_a\cong\left(\frac{du}{dx}\right)_0-\left(\frac{d^2u}{dx^2}\right)_0 b\cong\left(\frac{du}{dx}\right)_0-b\beta^2u(0) \tag{11・23}$$

$$=\left(\frac{du}{dx}\right)_0-\left(\frac{2P}{a}\right)u(0)$$

ここに P は (11・20) 式で定義されている．それで

$$\left[i(\alpha-k)-\left(\frac{2P}{a}\right)\right]A-\left[i(\alpha+k)+\left(\frac{2P}{a}\right)\right]B \tag{11・24}$$

$$=i(\alpha-k)Ae^{i(\alpha-k)a}-i(\alpha+k)Be^{-i(\alpha+k)a}$$

(11・22) 式と (11・24) 式の解が存在するための行列方程式は

$$\begin{vmatrix} 1-e^{i(\alpha-k)a} & 1-e^{-i(\alpha+k)a} \\ i(\alpha-k)(-e^{i(\alpha-k)a})-(2P/a) & -i(\alpha+k)(1-e^{-i(\alpha+k)a})-(2P/a) \end{vmatrix}=0$$

これを分解すれば容易に (11・21) 式を得る．

波動ベクトル帯の波動函数

読者はこの章でいくらか矛盾を感じられることと思う．すなわち前章では一価金属に対して自由電子近似が便利なことを強調し，この章では個々の原子の伸位やイオン殻と伝導電子との相互作用の重要性を強調しているからである．幸いなことに一価金属ではこの矛盾は単に見掛けのものに過ぎない．エネルギー・バンドのエネルギーは自由電子の場合とほとんど同じような形で波動ベクトルに依存するけれども波動函数の方は相当異っており，電荷は独立した原子のときと同様正のイオン殻に集積することもありうる．

前章の重要な結果によれば，自由電子模型ではつぎの関係が成立する．

$$E_k=(\hbar^2/2m)k^2 \tag{11・25}$$

ここで見方を拡張し，エネルギーが波動ベクトルの二乗に比例する点を重視することにする．そしてこの比例係数が変ってもよいということにする．すなわち

$$E_k=(\hbar^2/2m^*)k^2 \tag{11・26}$$

ここに m^* は有効質量とよばれる．そしてとりわけフェルミ・エネルギー，比熱，帯磁率，伝導度などの m に単に m^* を代入してもよかろうと考える．

最初まず波動函数が平面波でないのに $E_k\cong(\hbar^2/2m)k^2$ とするとどうなるかを調べてみよう．まず周期ポテンシャル内における $\mathbf{k}=0$ に対する波動函数は解けているものと考える．この解は $\psi=u_0(\mathbf{r})$ でここに $u_0(\mathbf{r})$ は格子の周期をもち，その形はイオンの中心付近のポテンシャルエネルギーの変化を反映しているであろう．つぎの函数を作ってみる．

$$\psi=u_0(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{11・27}$$

この函数は (11・3) 式のブロッホの形をもっているが，u が $\mathbf{k}$ の函数であることを無視しているから，一般に波動方程式の正確な解ではない．しかしこれは正しい函数に対しては平面波よりはずっとよい近似のはずである．この近似解は $u_0(\mathbf{r})$ であらわされる変調を強くうけているけれども，そのエネルギーは $\mathbf{k}$ に対して $(\hbar^2/2m)k^2$ の形をしており，平面波と全く同一である．つぎのようにしてエネルギーの平均値を計算しよう．量子力学の平均値を求める方法により

$$\overline{E}=\int u_0^*(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right]e^{i\mathbf{k}\cdot\mathbf{r}}u_0(\mathbf{r})d\tau \tag{11・28}$$

は

$$\nabla e^{i\mathbf{k}\cdot\mathbf{r}}u_0(\mathbf{r}) = i\,\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{r}}u_0(\mathbf{r}) + e^{i\mathbf{k}\cdot\mathbf{r}}\nabla u_0(\mathbf{r})$$

$$\nabla^2 e^{i\mathbf{k}\cdot\mathbf{r}}u_0(\mathbf{r}) = -k^2e^{i\mathbf{k}\cdot\mathbf{r}}u_0(\mathbf{r}) + 2i\,\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{r}}\nabla u_0(\mathbf{r}) + e^{i\mathbf{k}\cdot\mathbf{r}}\nabla^2 u_0(\mathbf{r})$$

をもちいて

$$\overline{E} = \frac{\hbar^2}{2m}k^2 + \int u_0^*(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]u_0(\mathbf{r})d\tau \tag{11・29}$$

$$= \frac{\hbar^2}{2m}k^2 + E_0$$

となる．$\int u_0^*(\mathbf{r})\nabla u_0(\mathbf{r})d\tau$ は対称性から零となる．なんとなれば $k=0$ に対し状態 u_0 は $\mathbf{r}$ の偶函数または奇函数であることが示されるからである．かくして望みの結果(11・29)式が得られた．

$u_0(\mathbf{r})$ は多くの場合単位胞の中の電荷分布をよくあらわすので，これの確かな計算の方法を得ることはきわめて興味深い．ウィグナーとサイツは簡単でしかも正確な $u_0(\mathbf{r})$ を，自由イオンの場がわかっているときに求める方法を発展させた．これはつぎにのべることにする．この方法が発表されて以来，固体内の波動函数を求めることについて数多くの発展があったが，本書では省略することにする．

ウィグナー・サイツの方法

ウィグナー・サイツ[6]の方法は体心立方と面心立方構造に最も簡単に適用される．これらの構造は，全空間を各原子とその最近接原子および（bcc では）次近接原子とを結ぶ線分の垂直二等分面で作られる多面体ですきまなく満すことができる．かくして得られた原子多面体を図 11・10 に示す．

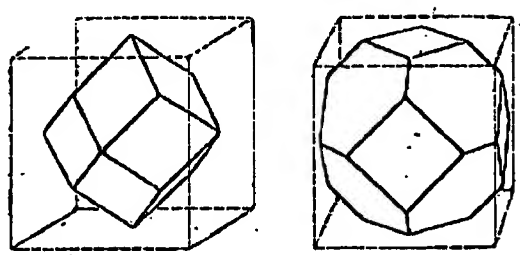


図 11・10 原子を包む原子多面体．(a) 面心立方 (b) 体心立方格子．まわりの立方体はともに両方の単位格子を示している

6) E.P., Wigner and F. Seitz, Phys. Rev. 43, 804 (1933); 46, 509 (1934).

イオン殻は各多面体の中心にある．Na^+ イオンのイオン半径は大体 0.95 Å であり，最近接原子間距離の半分が 1.85 Å あるという事実に注目しよう．すると原子多面体内の大部分の体積にある伝導電子のポテンシャルエネルギーは小さく，またポテンシャルの大きいイオン殻の内側ではほとんど球対称である．かくして多面体のポテンシャルはよい近似で球対称であるとみることができる．

$k=0$ の波動函数は格子の周期をもち，その上格子点につき対称である．この二つの条件を満足させるためには，各多面体の面上の垂直な微分係数 $\partial u_0/\partial n$ が零でなければならない．多面体は実際には球で近似してもそう悪くなく，ウィグナーとサイツは s 球とよばれる球で近似した．球の半径 r_0 は原子多面体と同体積という条件からきめられるので bcc 構造では，a を格子定数とすれば

$$\frac{4\pi}{3}r_0^3 = \frac{1}{2}a^3$$

から定まる．すなわち

$$r_0 = (3/8\pi)^{1/3}a \cong 0.49\,a \tag{11・30}$$

原子多面体上の境界条件 $\partial u_0/\partial n = 0$ は，したがって S 球上の簡単なつぎの条件で置き換えられる．

$$(\partial u_0/\partial r)_{r_0} = 0 \tag{11・31}$$

したがって問題はこの近似を用い，(11・31) 式の境界条件で

$$\left[-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) + V(r)\right]\psi = E\psi \tag{11・32}$$

を解くことに帰着する．ここに $V(r)$ はイオン殻のポテンシャルで，これは自己無撞着の方法か，または分光学的に定めた自由原子のエネルギー単位に経験的に合わせるようにして定める．(11・32)式を解いて求めた金属ナトリウムの (3s) 伝導バンドの最底状態の波動函数を図 11・11 に示してある．波動函数は原子容積のうち 90％くらいはほとんど一定であることを注意しよう．(11・27) 式に示すように k の大きい方の解が $e^{i\mathbf{k}\cdot\mathbf{r}}u_0(\mathbf{r})$ で近似される範囲では，伝導バンドの波動

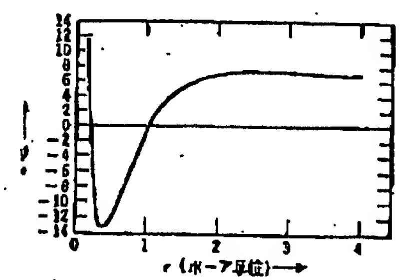


図 11・11 金属ナトリウムの最低エネルギー状態の波動函数，1 ボーア単位は 0.529×10^{-8} cm．

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